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Phase transitions in the steady state behavior of mechanically perturbed spin glasses and ferromagnets

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We analyze the steady state regime of systems interpolating between spin glasses and ferromagnets under a tapping dynamics recently introduced by analogy with the dynamics of mechanically perturbed granular media. A crossover from a second order to first order ferromagnetic transition as a function of the spin coupling distribution is found. The flat measure over blocked states introduced by Edwards for granular media is used to explain this scenario. Annealed calculations of the Edwards entropy are shown to qualitatively explain the nature of the phase transitions. A Monte-Carlo construction of the Edwards measure confirms that this explanation is also quantitatively accurate.

PACS: 05.20 y Classical statistical mechanics, 75.10 Nr Spin glasses and other random models, 81.05 Rm Porous materials; granular materials

In complex systems such as granular media the energy available due to thermal fluctuations is not sufficient to cause particle rearrangement, hence in the absence of external perturbations the system is trapped in a metastable state. A granular media may be shaken mechanically and experiments reveal a steady state regime defined by an asymptotic density [1]. The non trivial behavior of these systems, such as slow relaxation dynamics and hysteresis effects arises from the fact that such systems have an extensive entropy of metastable or blocked states. A vertically tapped system of hard spheres tends to a random close packing [1], whereas a horizontally shaken system crystallizes [2], the stationary states obtained in these systems are not theoretically understood for the moment. Edwards [3,4] has proposed that one may construct a thermodynamics over metastable states in the same way as Boltzmann and Gibbs developed over microstates, his hypothesis is that the equilibrium measure is flat over all blocked or metastable states satisfying the relevant macroscopic constraints. This is an ergodic hypothesis which is conceivably true in the case of *extensive manipulations* such as stirring, pouring, shaking an tapping. This scenario had been recently tested on a wide range of models by comparing dynamical time averaged quantities in the steady state with those predicted by a flat measure which is either calculated numerically or analytically [5–7]. In a number of systems the Edwards measure was seen to work extremely well, although, reassuringly given the strength of the hypothesis, there are cases where it does not appear to be applicable [5].

Given the recent interest in the Edwards measure and the fundamental and industrial importance of mechanically driven systems it is natural to examine phase transitions in this context. As pointed out by Edwards and coworkers, the construction of a steady state measure for mechanically perturbed systems would allow one to predict, for example, whether two powders or granular media form a mixture or phase separate upon stirring or shaking. In mean field implementations of the Edwards measure to binary granular systems second order phase transitions have been found between the mixed and separated phases [4].

Recently [6] there has been interest in using spin systems to examine tapping like dynamics on systems with an extensive entropy of metastable states. These systems, though far from being realistic models of granular media, provide a testing ground for the development of thermodynamic like theories for granular systems and indeed seem to show much of the phenomenology seen in real systems.

The models we shall consider are Ising spin systems on random thin graphs. A random thin graph is a collection of N points, each point being linked to exactly c of its neighbors, c therefore being the connectivity of the graph. The spin glass/ferromagnet model we shall consider has the Hamiltonian $H = -\frac{1}{2}\sum_{j\neq i} J_{ij} n_{ij} S_i S_j$ where the S_i are Ising spins, n_{ij} is equal to one if the sites i and j are connected and zero otherwise. The fact that the local connectivity is fixed as c imposes the local constraints $\sum_j n_{ij} = c$, for all sites i. For the following, we have fixed $c = 3$. The couplings J_{ij} are independent random variables with distribution: $P(J_{ij}) = \alpha\delta(J_{ij}+1) + (1-\alpha)\delta(J_{ij}-1)$ (α being a parameter in $[0, 1/2]$).

We define the tapping dynamics as follows: In between the taps, the system has a natural zero temperature relaxational dynamics, it evolves under a random sequential single spin flip dynamics where only moves which reduce the energy are allowed. When blocked, it is tapped with strength $p \in [0, 1/2]$, that is to say each spin is flipped with a probability p, the updating at this point being parallel - this corresponds to the extensive manipulation. The system is then evolved by the zero temperature dynamics until it becomes once again stuck and

the tapping is repeated. After a transient regime, the system reaches a stationary regime characterized by an energy per spin $E(p)$. Numerical simulations show that $E(p)$ is a monotonically decreasing function of p - the lighter one taps, the lower the energy obtained. Here we make the analogy with experiments on vertically tapped granular media [1], where (in the reversible part of the experiment) the asymptotic compactivity increases as the system is more lightly tapped. Our numerical simulations are reversible and one can move up and down the curve of $E(p)$ if the system is tapped for a sufficiently long time after changing p. Here the macroscopic quantity which is fixed on average by the tapping dynamics is $E(p)$, whereas in granular material it is the average volume $v = V/N$ per particle.

The canonical form of the Edwards hypothesis [7,8] then leads to the consideration of the partition function $Z(\beta) = \int dE\, dm\, \exp\left(-N(\beta E - s_{Edw}(E,m))\right)$, where $s_{Edw}(E,m)$ the Edwards entropy per spin at average energy E and magnetization m per spin. Here $\beta = \beta(p)$ is a Lagrange multiplier fixing E, numerical tapping simulations thus suggest that $\beta(p)$ decreases as p is increased. In spin glasses the Edwards entropy per spin at fixed average energy can be calculated (or approximated) and can be shown to be extensive (*i.e.* $s_{Edw}(E)$ is of order 1 and independent of N in the thermodynamic limit). As mentioned previously granular systems are expected to share this property. Let us emphasize at this point that this rather ambitious goal of developing a thermodynamics for granular systems does use additional information about the dynamics as compared to usual thermodynamics. The definition of the entropy contains the information about metastability. This is a partial, though rather limited, use of dynamics to describe statics.

If we assume that $\beta(p)$ is continuous on reducing p one expects the possibility of an onset of ferromagnetic ordering, which would correspond to phase separation in a granular material. The Edwards free energy per spin $f(\beta) = \min_{E,m} f(E,m,\beta) = \min_E f(E,\beta)$ with $f(E,m,\beta) = E - s_{Edw}(E,m)/\beta$ and $f(E,\beta) = f(E,m(E),\beta)$, where $m(E)$ is the point where $f(E,m,\beta(p))$ is a minimum with respect to m. The value of $m(E)$ is thus given by $\partial s_{Edw}(E,m(E))/\partial m = 0$. In the models studied here we find that there exists a value E_c such that for $E > E_c$ one has $m(E) = 0$ and for $E < E_c$ the solution $m = 0$ becomes a local maximum of $f(E,m,\beta)$ and there is a second order phase transition with m becoming non zero.

For $E < E_c$ in the neighborhood of E_c we have found that, depending on the parameters of the disorder, there are two possible behaviors:

(1) $\partial^2 s_{Edw}(E,m(E))/\partial E^2|_{E=E_c^-} < 0$ in which case the ferromagnetic phase is stable and the system exhibits a second order phase transition in the energy with a discontinuity in $\partial\beta/\partial E$.

(2) $\partial^2 s_{Edw}(E,m(E))/\partial E^2|_{E=E_c^-} > 0$ and the ferromagnetic phase is unstable. In this case there is a second minimum of $f(E)$ (case (2a)) or end point of $f(E)$ (where the Edwards entropy vanishes, that is to say the ground state E_{GS}) (case (2b)) at an energy E^* which is strictly lower than E_c. Hence there is a first order phase transition with a non zero spontaneous magnetization $m(E^*)$. We find in this case that the paramagnetic phase may be in fact only metastable for a range of values $\beta < \beta_c$ *i.e.* the second minimum exists below β_c and may have a lower Edwards free energy. Comparing our simulations with the annealed calculation we find it is only when this metastable phase becomes unstable (at the spinodal point) that the transition occurs. This suggests that the tapping dynamics is not efficient at tunneling over free energy barriers - it is interesting to note that the fluffy (arch rich) phase in granular media exhibit this strong metastability [1].

With respect to the relaxational part of the dynamics introduced above, the total number of metastable states for a given set of J_{ij} and n_{ij} is given by :

$$N_{MS}(E,m) = \mathrm{Tr} \prod_{i=1}^{N} \theta\left(\sum_{j\neq i} J_{ij} n_{ij} S_i S_j\right) \delta(H - NE)\, \delta(\sum_i S_i - Nm) \qquad (1)$$

where $\theta(x) = 0$ if $x < 0$ and $\theta(x) = 1$ if $x \geq 0$. The above formula expresses the fact that each spin is aligned with its local molecular field in a metastable state and hence none can flip under the relaxational dynamics. The Edwards entropy of the metastable states of energy per spin E and at magnetization m is thus $s_{Edw}(E,m) = \frac{1}{N}\langle\langle \ln N_{MS}(E,m)\rangle\rangle$, the brackets denoting the average over the disorder. Unfortunately this average is not easily taken analytically at low energy, and we have to compute an annealed average, which will give an upper bound for the Edwards entropy:

$$s_{Edw}(E,m) = \lim_{N\to\infty} \frac{1}{N} \ln\langle\langle N_{MS}(E,m)\rangle\rangle \qquad (2)$$

In the the SK model [11] and for Ising spin systems on random thin graphs [9], there exists an energy E_{ann} above which this annealed approximation is exact.

The computation of this quantity is a generalization of that for $\alpha = 0$ [9]. One finds $s_{Edw}(E,m)$ is given by the saddle point value of the action

$$\begin{aligned} S(u,v,t,\beta;E,m) = -\beta\left(\tfrac{c}{2} - E\right) + \tfrac{c}{2}\ln(1-2\alpha) \qquad (3)\\ - \tfrac{c}{2}\ln\left[(1-\alpha)(2t+u^2+t^2v^2) - \alpha(2tuv+1+t^2)\right]\\ + \tfrac{1+m}{2}\ln\left(f(ue^{\beta})\right) + \tfrac{1+m}{2}\ln\left(t^c f(ve^{\beta})\right)\\ - \tfrac{1+m}{2}\ln\left(\tfrac{1+m}{2}\right) - \tfrac{1-m}{2}\ln\left(\tfrac{1-m}{2}\right) \end{aligned}$$

with respect to the parameters u, v, t and β. The magnetization of the metastable states at energy E is given by the maximization of (3) with respect to m:

$$m = \frac{f(ue^{\beta}) - t^c\, f(ve^{\beta})}{f(ue^{\beta}) + t^c\, f(ve^{\beta})} \qquad (4)$$

In order to compute the Edwards entropy, we solve the stationarity conditions coming from the extremization with respect to u, v, t, β of $S(u, v, t, \beta; E, m(E))$, with $m(E)$ replaced by the expression (4). The resulting value for β is $\beta = \frac{\partial s_{Edw}(E)}{\partial E}$, which is the definition of the inverse Edwards temperature.

The saddle point can be found numerically to compute $f(E, \beta)$. In the annealed approximation when $\alpha < \alpha_c \simeq 0.06$ we find that we are in scenario (2), for $\alpha > \alpha_c$ we are in scenario (1). Shown in Figs. (1), (2) and (3) is the behavior of $f(E, \beta)$ for $\alpha = 0$, $\alpha = 0.04$ and $\alpha = 0.12$ respectively and one sees that one has the behaviors (2b), (2a) and (1). In the range $\beta_0 < \beta < \beta_c$ shown in Figs. (1) and (2) the higher energy, paramagnetic, minimum is only metastable.

To test the above predictions, we have tapped systems with $\alpha = 0.002, 0.005, 0.02, 0.05$ and recorded both the energy $E(p)$ and the magnetization $m(p)$ in the quasi equilibrium regime. Systems were of size $N = 10^6$ and we have checked that this was large enough to consider a single sample instead of several realizations of disorder. The curves for $E(p)$ are shown in Fig. (4). For $\alpha = 0.005$ and $\alpha = 0.002$, there is a first order phase transition, whereas for $\alpha = 0.05$ and $\alpha = 0.02$ this transition is a second order one, in qualitative agreement with the previous discussion of the role of the Edwards entropy. Of course, as the annealed entropy is not expected to be exact a low energy, the values of α_c and $E_c(\alpha)$ which come from this calculation are only approximate. Indeed, it is found in the tapping simulations that $0.005 < \alpha_c < 0.02$, and $E(p_c(\alpha)^+, \alpha)$ differs systematically with $E_c(\alpha)$ found from Eq. (2).

In order to test this scenario in a quantitative fashion, we have computed the Edwards entropy as was done in [5]. One introduces an auxiliary temperature $1/\beta_{aux}$, which is a Lagrange multiplier to fix the number of spins which are not in the same direction as their local field. Then, one fixes β and does a Monte-Carlo simulation using the Metropolis algorithm where a randomly chosen spin is flipped with probability $\min\left(1, e^{-\beta_{aux}\Delta\mathcal{H}_{aux}}\right)$, with $\beta_{aux}\mathcal{H}_{aux} = \beta\mathcal{H} + \beta_{aux}\sum_i \theta\left(s_i \sum_{j\neq i} n_{ij} J_{ij} s_j\right)$. Starting from $\beta_{aux} = 0$, we increased it very slowly until the system was blocked in a metastable state. Repeated several times, this allowed us to sample $E(\beta)$ for systems of $N = 10^5$. At the end of the simulation, we have recorded both energy and magnetization. The comparisons between $m(E(p))$ from tapping simulations and $m(E(\beta))$ from Monte-Carlo simulations for $\alpha = 0.05$ are shown in Fig.(5), the agreement is excellent. In the high temperature region $\beta \in [0, \beta_c(0)]$, for all $\alpha \in [0, 1/2]$, the value of $E(\beta)$ measured in the simulations were in excellent agreement with the results of the annealed calculation, indicating the latter is correct in this range. For $\beta_c(0) < \beta < \beta_c(\alpha)$ (here we mean β_c from the annealed approximation) the annealed calculation is close but certainly deviates from the numerically measured one (see Fig (6)). Moreover, the value of $E_c(\alpha)$ found in this Monte-Carlo procedure was much closer to $E(p_c(\alpha)^+)$ than that found in the annealed approximation. This means that this approximation is not exact for E when $m(E) \neq 0$ and explains the quantitative disagreement between $E(p_c(\alpha)^-, \alpha)$ and $E^*(\alpha)$ obtained from (3).

For $\alpha < \alpha_c$, the simulated annealing again predicts $E_c(\alpha)$ very close to $E(p_c(\alpha)^+, \alpha)$ determined by the tapping simulations. The behavior of the low energy magnetization for $E < E^*(\alpha)$ is also the same for the two simulations, although the region of energy close to $E^*(\alpha)$ is difficult to sample with the simulated annealing. Fig.(7) is the histogram of the energy obtained during the tapping dynamics in the stationary regime for $\alpha = 0.002$ for different p near p_c, for a relatively small system size. There are clearly two peaks separated by a gap and the spread towards negative energy of the one of highest energy becomes large when p approaches p_c, thus indicating the approach of the spinodal point. It is interesting to compare Fig. (2) qualitatively with Fig.(7), the comparison is quite striking. For β slightly smaller than β_c we see that the form of the high energy peak, with a small spread to the right and a large one to the left is predicted by the geometry of the first minimum of $f(E, \beta)$ in Fig. (2). In addition for β slightly smaller than β_c we see that the ferromagnetic minimum is close to its spinodal point, thus explaining the large, two sided in this case, spread in the histogram in this region.

In conclusion we have examined a dynamics driven by an extensive external perturbation on a family of systems having an extensive Edwards entropy of blocked states. The existence of first and second order ferromagnetic transitions are qualitatively explained by invoking the Edwards measure calculated within an annealed approximation. The quantitative predictions using this measure in Monte-Carlo simulations are also in excellent agreement with tapping simulations on the system. We have found similarly promising results in models of higher connectivity and in the infinitely connected SK spin glass [12]. This work suggests the possibility of using the Edwards measure to explain phase transitions in realistic granular systems, the main obstacle is the technical difficulty in the computation of the Edwards measure.

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Figure captions

Fig. 1. Free energy $f(E,\beta)$ versus E for different values of β with $\alpha = 0$. Between A and B, the local minimum has the lowest free energy, between B and C, it is only metastable and above C it is no longer a minimum.

Fig. 2. Free energy $f(E,\beta)$ versus E for different values of β and $\alpha = 0.04 < \alpha_c$. One sees that when β increases the minimum of high energy starting as a global minimum becomes metastable and then disappears at the transition.

Fig. 3. Free energy $f(E,\beta)$ versus E for different values of β and $\alpha = 0.12 > \alpha_c$. Here there is only one local minimum which moves continuously with β. The vertical dashed lines indicates the energy E where $f(E,\beta)$ is non analytic.

Fig. 4. Energy per spin $E(p)$ in the steady state regime versus p for $\alpha = 0.002, 0.005, 0.02, 0.05, 0.5$ and $N = 10^6$ spins.

Fig. 5. Comparison of the measurements of $m(E)$ in the tapping simulations and Monte-Carlo simulations. In the former (a) $m(p)$ is plotted versus $E(p)$ and in the latter (b) $m(\beta)$ is plotted versus $E(\beta)$.

Fig. 6. Comparison of $E(\beta)$ for $\alpha = 0.05$ obtained from the annealed calculation (a) and the Monte-Carlo simulation (b). At the right of the vertical dashed line, the annealed calculation is not exact any more. It predicts a first order phase transition, whereas the Monte Carlo predicts a second order one, with E_c in very good agreement with that of the tapping at $p = 0.05$.

Fig. 7. Histogram of the energy during the tapping simulations in the steady state regime for $\alpha = 0.002$ and $N = 25000$ spins during 10^5 taps and for $p = 0.2584, 0.2585, 0.2586, 0.2587, 0.2588, 0.2589$ (reading left to right from the top).

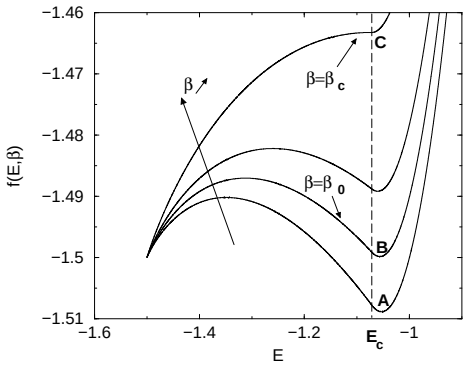

FIG. 1.

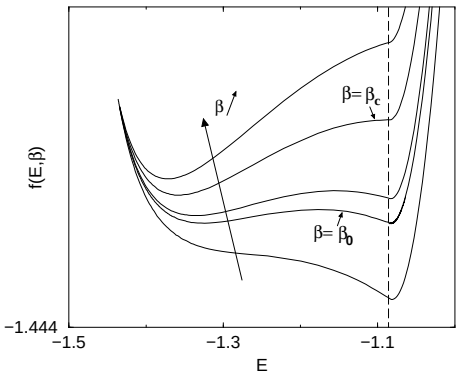

FIG. 2.

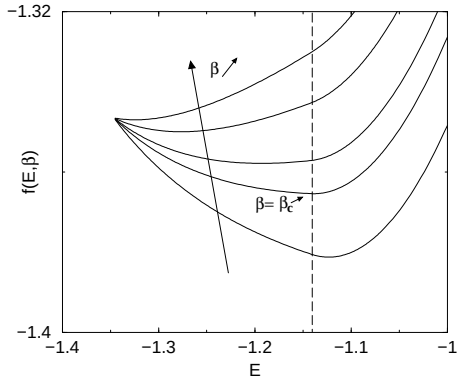

FIG. 3.

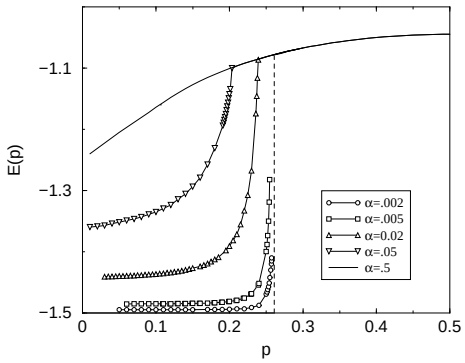

FIG. 4.

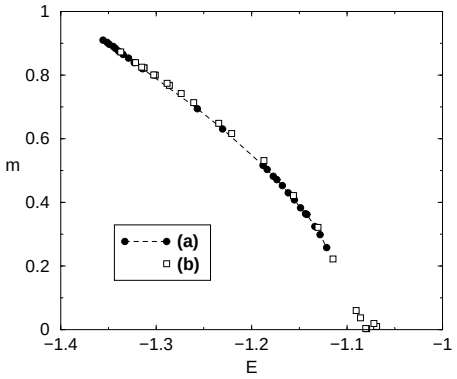

FIG. 5.

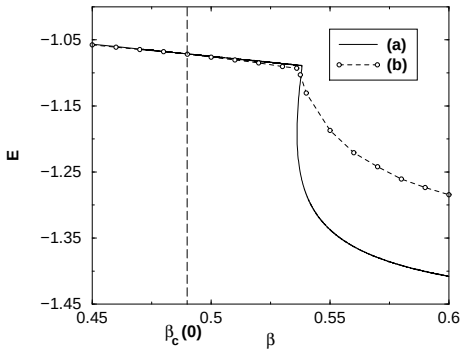

FIG. 6.

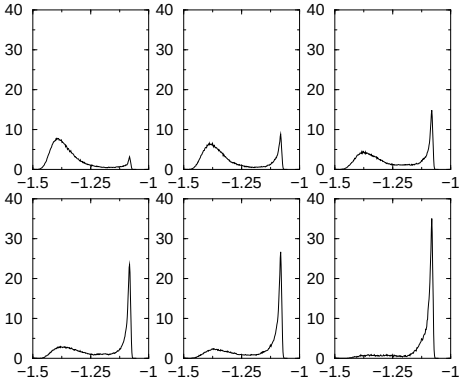

FIG. 7.